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TOPAZ3D - A three-dimensional finite element heat transfer code

Arthur B. Shapiro

August, 1985

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TOPAZ3D - A three-dimensional finite element heat transfer code



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August, 1985

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TOPAZ3D - A three-dimensional finite element heat transfer code

1. INTRODUCTION

TOPAZ3D is a three-dimensional implicit finite element computer code for heat transfer analysis. This report provides a user's manual for TOPAZ3D and a description of the numerical algorithms used. Sample problems with analytical solutions are presented. TOPAZ3D has been implemented on the CRAY and VAX computers.

TOPAZ3D can be used to solve for the steady state or transient temperature field on three dimensional geometries. Material properties may be temperature dependent and either isotropic or orthotropic. A variety of time and temperature dependent boundary conditions can be specified including temperature, flux, convection and radiation. By implementing the user subroutine feature, users can model chemical reaction kinetics and allow for any type of functional representation of boundary conditions and internal heat generation. TOPAZ3D can solve problems of diffuse and specular band radiation in an enclosure coupled with conduction in the material surrounding the enclosure. Additional features include thermal contact resistance across an interface, bulk fluids, phase change and energy balances. Thermal stresses can be calculated using the solid mechanics code NIKE3D [1] which reads the temperature state data calculated by TOPAZ3D.

TOPAZ3D has no general mesh generation capability. Rows of evenly spaced nodes and rows of sequential elements may be generated. For complex zoning, the mesh generation code and preprocessor INGRID [2] should be used. The TAURUS [3] interactive post-processor can be used to provide temperature contour, temperature-time history and various geometry plots.

TOPAZ3D is an extension of the two dimensional heat transfer code TOPAZ [4] to three dimensions. TOPAZ3D is based to some extent on work by W.E. Mason and P. J. Burns in developing TACO3D [5]. S.J. Sackett has been influential in the development of TOPAZ3D by writing the bandwidth and profile minimization routines [6], the equation solver FISSLE [7] and many utility routines.

2. GENERAL THEORY

Conduction of Heat in an Orthotropic Solid

The differential equation of conduction of heat in a three-dimensional solid is given by

$$\rho c \frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x} \left[k_x \frac{\partial \theta}{\partial x} \right] + \frac{\partial}{\partial y} \left[k_y \frac{\partial \theta}{\partial y} \right] + \frac{\partial}{\partial z} \left[k_z \frac{\partial \theta}{\partial z} \right] + q_g \quad \text{in } \Omega$$
 (1)

subject to the boundary condition

$$k_x \frac{\partial \theta}{\partial x} n_x + k_y \frac{\partial \theta}{\partial y} n_y + k_z \frac{\partial \theta}{\partial z} n_z + \beta \theta = \gamma$$
 on Γ (2)

and with the initial condition

$$\theta = \theta (x,y,z) \quad \text{at } t = t_0 \quad . \tag{3}$$

Equations (1)-(3) represent the strong form of a boundary value problem to be solved for the temperature field within the solid.

TOPAZ3D employs essentially the same theory as TOPAZ in solving Eq. (1) by the finite element method. Those interested in a detailed description of the theory are referred to the TOPAZ [4] user's manual. TOPAZ3D uses an 8 node trilinear hexahedral element for spatial discretization of the geometry. The hexahedral element can degenerate to a 6 node triangular prism and a 4 node tetrahedron. These elements are integrated with a 2x2x2 Gauss quadrature rule, with temperature dependence of the properties accounted for at the Gauss point. Time integration is performed using a generalized trapezoidal method shown by Hughes [8] to be unconditionally stable for nonlinear problems. Fixed point iteration with relaxation is used to satisfy equilibrium in nonlinear problems.

The finite element method provides the following equations for the numerical solution of Eqs. (1)-(3).

$$\begin{bmatrix} \frac{C}{n+\alpha} + \alpha H_{n+\alpha} \end{bmatrix} \{ \theta_{n+1} - \theta_n \} = \{ F_{n+\alpha} - H_{n+\alpha} \theta_n \}$$

$$[C] = \sum_{e} [C_{ij}^e] = \sum_{e} \int_{\Omega} N_i \rho c N_j d\Omega$$

$$[H] = \sum_{e} [H_{ij}^e] = \sum_{e} \left[\int_{\Omega} \nabla^T N_i K \nabla N_j d\Omega + \int_{\Gamma} N_i \beta N_j d\Gamma \right]$$

$$[H] = \sum_{e} [H_{ij}^e] = \sum_{e} \left[\int_{\Omega} N_i q_g d\Omega + \int_{\Gamma} N_i \gamma d\Gamma \right]$$

$$[F] = \sum_{e} \{ F_i^e \} = \sum_{e} \left[\int_{\Omega} N_i q_g d\Omega + \int_{\Gamma} N_i \gamma d\Gamma \right]$$

$$N_i (\xi, \eta, \zeta) = \frac{1}{8} (1 + \xi_i \xi) (1 + \eta_i \eta) (1 + \xi_i \zeta)$$

The parameter α is taken to be in the interval [0,1]. Some well known members of this α -family are

<u>a</u>	<u>Method</u>
0	forward difference; forward Euler
1/2	midpoint rule; Crank-Nicolson
2/3	Galerkin
1	backward difference

3. ASPECTS OF TOPAZ3D

The sections in this chapter should be consulted prior to and during the construction of a TOPAZ3D input deck. Many helpful suggestions, warnings and procedural information are contained in each section.

3.1 Bandwidth Minimization

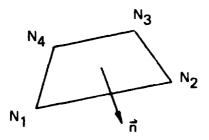
The Gibbs-Poole-Stockmeyer algorithm [6] coded by S. J. Sackett is available as an option in TOPAZ3D to minimize the bandwidth and profile of the conductance matrix. The result of bandwidth minimization is a decrease in computer memory requirements. The bandwidth should always be minimized for transient problems. However, for steady state problems, the cpu time required for bandwidth minimization may be greater than the time to solve the problem with the unminimized bandwidth. For steady state problems, I recommend minimizing the bandwidth only if computer memory requirements are excessive. Bandwidth minimization node renumbering is transparent to the user. All calculated nodal quantities are printed using the user's original node numbering scheme.

3.2 Boundary Conditions

Boundary conditions are represented by

$$k_x \frac{\partial \theta}{\partial x} n_x + k_y \frac{\partial \theta}{\partial y} n_y + k_z \frac{\partial \theta}{\partial z} n_z = \gamma - \beta \theta = q^{"}$$

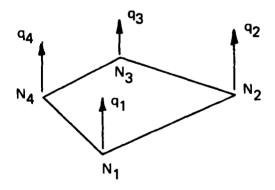
By convention heat flow is positive in the direction of the surface outward normal vector. Surface definition is in accordance with the right hand rule. The outward normal vector points to the right as one progresses from node N_1 - N_2 - N_3 - N_4 .



Boundary conditions can be functions of temperature or time. More than one boundary condition can be specified over the same surface such as in a case of combined convection and radiation. For situations where it is desired to specify adiabatic (i.e. $\dot{q}''=0$) conditions such as at an insulated surface or on a line of symmetry, no boundary condition need be specified. This is the default boundary condition in TOPAZ3D.

<u>Temperature</u>. Temperature boundary conditions can be specified on any node whether on the physical boundary or not.

Flux. Set $q'' = q_f$ where q_f is defined at the node points comprising the flux b.c. surfaces.



<u>Radiation</u>. A radiation boundary condition is calculated using a radiant-heat-transfer coefficient. Set $\dot{q}'' = h_r (T-T_{\infty})$, where h_r is a radiant-heat-transfer coefficient defined as

$$h_r = \sigma \mathcal{F} (T + T_{\infty}) (T^2 + T_{\infty}^2) .$$

The exchange factor, \mathcal{F} , is a characterization of the effect of the system geometry, emissivity and reflectivity on the capability of radiative transport between surfaces. The radiation b.c. data cards require specification of the product, $f = \mathcal{F} \sigma$, and T_{∞} for the boundary surface.

Convection. Set
$$\dot{q}'' = h(T-T_{\infty})^a (T-T_{\infty})$$

where

h heat transfer coefficient.

 $(T-T_{\infty})^a$ free convection temperature dependence.

 $(T-T_{\infty})$ temperature potential.

For forced convection calculations set a=0. Then \dot{q}'' = h (T - T $_{\infty}$). For free convection calculations empirical formulas are available to calculate the heat transfer coefficient. These formulas contain the Grashof

number raised to some power, a. For example, the average value of the heat transfer coefficient for laminar free convection from an isothermal vertical plate of length L is

$$h = \frac{0.555 \text{ k } \text{Pr}^{1/4} \text{Gr}_{L}^{1/4}}{L}$$

where the Grashof number is

$$Gr_L = \frac{\rho^2 g \beta (T-T_{\infty}) L^3}{\mu^2}$$

The rate of heat transfer by convection between the plate and a fluid may be computed by the relation

$$q'' = h(T-T_m)$$

$$= 0.555 \frac{k}{L} \left(\frac{Pr \ p^2g \ \beta L^3}{12} \right)^{1/4} (T-T_{\infty})^{1/4} (T-T_{\infty}) .$$

The term

$$0.555 \frac{k}{L} \left(\frac{Pr \rho^2 g L^3}{\mu^2} \right)^{1/4}$$

contains constants and material properties which may be a function of temperature. Let h on the convection boundary condition data card represent this term. Give the free convection exponent, a, on this data card a value of 0.25 to account for the term

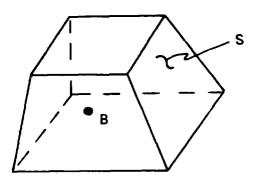
$$(T-T_{\infty})^{1/4}$$
.

TOPAZ3D evaluates h at the film temperature

$$T = \frac{1}{2} \left(T_{SURF} + T_{\infty} \right) .$$

3.3 Bulk Fluid

The bulk fluid concept is best described with the aid of the following figure:



Here a bulk node "B" is used to represent the entire volume of a particular material such as a gas in a cavity. The heat flow between the bulk node (material) "B" and an adjoining surface "S" is given by

$$\dot{q}$$
 = f(θ ,t) $(\theta_S^a - \theta_B^a)^b$

where θ_S and θ_B represent the temperatures of the surface "S" and the bulk node "B" respectively. In addition, the density, specific heat and volume of the bulk material are specified.

TOPAZ3D requires that a bulk node be given a node number as well as coordinates. However, these coordinates are arbitrary.

The bulk node concept can also be used in the case where it is desired to specify a lumped heat capacity at a node. In such a case, no surfaces "S" are associated with the bulk node and only the density, heat capacity and volume associated with the bulk node are specified.

3.4 Chemical Kinetics

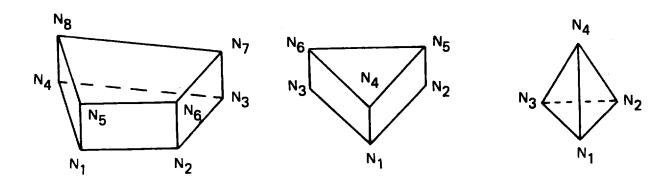
Subroutines have been developed for several types of reactive kinetics (e.g. thermite burns, high explosive detonations). These subroutines and instructions on their use may be obtained from the author.

3.5 Controller (thermostat) Options

Controlling the application of a boundary condition, such as a surface heat flux, as a function of a remote nodal temperature is handled through a special user subroutine. These subroutines and instructions on their use may be obtained from the author.

3.6 Element Types

An eight node trilinear hexahedral element is used. This element degenerates to a 6 node triangular prism and a 4 node tetrahedron as shown.



3.7 Energy Balances

Various energy terms are printed and written into the plot file for post processing using the code TAURUS [3]. The energy terms are:

- change in material internal energy for time step,
- change in material internal energy from initial time,
- heat transfer rates on boundary condition surfaces,
- heat transfer rates on enclosure radiation surfaces,
- x, y and z fluxes at all nodes.

3.8 Function Definitions

Any specified function of time or temperature (i.e., internal heat generation, boundary conditions) can be described by either a piecewise linear curve or by a functional relationship defined in a user subprogram. Functions that are dependent upon both time and temperature must be defined by a User Subprogram.

A typical piecewise linear curve is shown below.



Values of a function at intermediate points on a curve are obtained by linear interpolation. Functional values outside the range of a curve results in an error message and problem termination. (See Section 3.18 Restart Capability.)

A single curve may be used for several functions if their ordinates differ by only a constant. This is accomplished by the use of curve multipliers which are applied to the ordinate of the curve.

In order to differentiate between a function of time and a function of temperature, the sign on the number assigned to the curve describing the function is used. For a time variation, the curve number is positive and for a temperature variation, the curve number is preceded by a negative sign. A curve number of zero indicates that a function is constant.

3.9 Heat Generation

Volumetric heat generation rates may be specified by element, by material, or both (in which case the effect is additive). Volumetric heat generation rates can be functions of time or temperature (see Section 3.8).

3.10 Initial Conditions

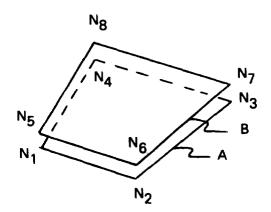
Initial temperature conditions can be specified on the nodal data input cards or on the nodal temperature initial condition cards. If no temperatures are specified, the default is 0. For nonlinear steady state problems the temperature initial condition serves as a first guess for the equilibrium iterations (see Section 3.14).

3.11 Special Internal Elements

Special internal elements allow thermal coupling between two surfaces (e.g. across a gap between two parts) according to the formula

$$q = f(\theta,t) (\theta_A^a - \theta_B^a)^b$$
.

The subscripts A and B refer to the element surfaces as indicated in the following figure.



 θ_A and θ_B are the respective average temperatures of these surfaces. Energy transport is normal to surface A. Surfaces A and B should be approximately the same area. While eight node numbers are required to define this element, opposed nodal coordinates may coincide. That is, an element may have zero thickness. This element is suitable for specifying contact

resistances between surfaces and for describing certain types of gaps between surfaces.

3.12 Material Properties

Heat capacity and thermal conductivity may be functions of temperature. Since the density and heat capacity appear only as a product in the governing equations, the temperature dependence of the density may be included in the temperature dependence of the heat capacity. Material properties are evaluated at the element Gauss point temperature.

The thermal conductivity may be either isotropic or orthotropic. For an orthotropic material, the three material axes (x_1', x_2', x_3') are orthogonal and the thermal conductivity tensor K' is diagonal.

The thermal conductivity tensor K in the global coordinate system (x_1, x_2, x_3) is related by

$$K_{i,j} = K'_{i,j} \beta_{mi} \beta_{n,j}$$

where

$$\beta_{ij} = \cos(x_i, x_j)$$

3.13 Mesh Generation

TOPAZ has no general mesh generation capability. Rows of evenly spaced nodes and rows of sequential elements may be generated. For complex zoning, the mesh generation code and pre-processor INGRID [2] should be used.

3.14 Nonlinear Analysis

In a nonlinear problem, C, H and F may be functions of θ and iteration is required to solve Eq. (4). Functional iteration with under relaxation is used. The nonlinear solution scheme consists of two steps. The first step called "reformation" is the assembly and triangularization of the coefficient matrix

$$\left[\frac{C_{n+\alpha}}{\Delta t} + \alpha H_{n+\alpha}\right] \tag{5}$$

in Eq. (4). This step is computationally expensive. The second step called an "equilibrium iteration" is the formation of the right hand side vector $\{F - H_{n+\alpha} \theta_n\}$ in Eq. (4) and back substitution to solve for $\{\theta_{n+1} - \theta_n\}$. This step is computationally inexpensive.

For strongly nonlinear problems (e.g. radiation boundary conditions) it is necessary to perform a reformation for each equilibrium iteration. For weakly nonlinear problems (e.g. material property nonlinearities) it is computationally advantageous to perform a reformation only at the beginning of the time step and then perform as many equilibrium iterations as required for convergence. Further still, a reformation of Eq. (5) can be performed and used over several time steps. The decision as to the number of reformations and equilibrium iterations is best to use on a particular problem must be made based on experience or a trial-and-error process.

In a steady state nonlinear problem, an initial guess should be made of the final temperature distribution and included in the input file as an initial condition. If your guess is good, a considerable savings in computation time is achieved.

3.15 Phase Change

A phase change algorithm developed by A. Edwards for the TRUMP code [9] has been implemented in TOPAZ. This algorithm explicitly constrains the solution of the conduction problem to satisfy phase change energy balance. Therefore, the finite element mesh and time step size for a specific analysis can be largely chosen by considering the accuracy predicted on the temperatures when phase changes are neglected. The phase change front may advance over several elements in a single time step.

A solution may show temperature oscillations at nodes near the phase change front. This is a result of the algorithm not following the phase change front but rather detecting phase change within an element and then lumping material latent heat at the nodes. Spacial discretization and time step size will effect the magnitude and decay rate of these temperature oscillations.

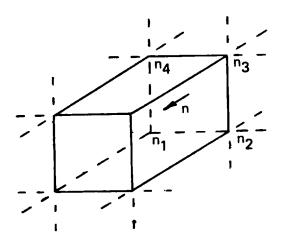
Phase change problems require specification of the problem as a nonlinear analysis and with backward difference time integration (α = 1). These conditions are automatically invoked on the analysis by setting the phase change calculation flag on control card one.

3.16 Post Processing

An interactive post processor TAURUS [3] is available to produce temperature contour plots, flux contour plots, temperature-time history plots, and various geometry plots. TAURUS can generate color plots.

3.17 Radiation in Enclosures

The theory and algorithms used for enclosure radiation problems is presented in the TOPAZ User's Manual [4]. An enclosure is defined by the discrete surfaces which are, in general, the boundaries of the finite elements which surround the enclosure as illustrated in the following figure.



The enclosure surfaces must be specified such that the surface outward normal vector points to the right as one proceeds from node $n_1-n_2-n_3-n_4$.

When an enclosure has an opening to the exterior of a body, the opening acts like a nonflective surface. Such a surface acts as a blackbody radiator (ε =1) at the outer surrounding temperature. Such surfaces are identified on the enclosure radiation data cards by flagging them as not participating in

the conduction part of the problem and giving them an emissivity curve number of zero.

Emissivity is input as a function of wavelength. If emissivity is considered not a function of wavelength, the first wavelength breakpoint λ , should be assigned a large number (e.g. 1 x 10^{10}). Note that the units on wavelength must be micrometers.

View factors can be calculated using the code FACET [10]. The code MONTE [11] can be used to calculate exchange factors for specular emitting and reflecting surfaces. Both these codes produce a view factor file for TOPAZ input.

Enclosure radiation problems can be expensive to solve both in computation time and computer core requirements. Problems using view factors that are not a function of wavelength are relatively quick because the $[\chi]$ matrix only has to be formed once for the problem. Problems using wavelength dependent emissivities are computationally slower because a Gauss-Seidel iterative solution is performed to solve the radiation part of the coupled problem for each wavelength band.

3.18 Restart Capability

For long transient problems, it is advisable to protect yourself by generating a "dump file" every so many time steps. These dump files along with a restart input deck will allow you to continue problem solution. This will protect you against.

- System crashes in which files are lost (assuming you were smart enough to save your dump files every so often).
- TOPAZ error terminations in which you are out of range on property curves or function curves.

The restart input deck allows the following parameters to be reset:

- final problem time,
- time step size,

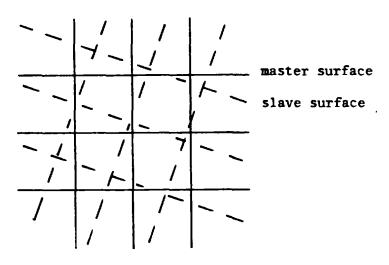
- output printing interval,
- output plotting interval,
- integration constant,
- nonlinear iteration parameters,
- material properties,
- function curves.

3.19 Steady State Analysis

TOPAZ3D has a one step steady-state solution algorithm. For nonlinear steady state problems iteration is required and an initial guess of the temperature field is needed. This can be specified on the initial temperature condition data cards.

3.20 Thermal Contact Resistance Across An Interface

Interface surfaces are defined to couple the finite element heat transfer equations between two parts through a thermal contact resistance across a gap between the contacting surfaces. The surfaces in contact can coincide spatially and have dissimilar zoning. One side of the contact surface is referred to as the master surface, and the other side is referred to as the slave surface. The designation of the slave and master surface is arbitrary. However, the surface which is more coarsely zoned should be chosen as the master surface. Each surface is defined by a set of 3 or 4 node quadrilateral surfaces called master and slave surfaces. Input for the algorithm requires that a list of master and slave surfaces be defined.



3.21 Thermal Stress Analysis

The temperatures calculated by TOPAZ3D can be used in performing uncoupled thermal stress analyses with the mechanical code NIKE3D [1]. This code can read the temperature states from the binary plot files generated by TOPAZ3D.

3.22 Transient Analysis

TOPAZ3D has both fixed and variable time step capabilities. The variable time step is limited to the range between a minimum and maximum time step that are input defined. Within this range, the time step is adjusted to limit the maximum temperature change in any element for the time step below a specified value.

3.23 Units

Any consistent set of units with the governing equations may be used. Examples are:

Quantity		Units	
temperature	K	c	F
space	m	cm	ft
time	S	S	hr
density	kg/m ³	g/cm ³	Lb _m /ft ³
heat capacity	J/kg K	cal/g C	Btu/Lb _m F
thermal conductivity	W/m K	cal/s cm C	Btu/hr ft F
thermal generation	W/m ³	cal/s cm ³	Btu/hr ft ³
heat flux	W/m ²	cal/s cm ²	Btu/hr ft ²

3.24 User Subprogram

A user subprogram option is available in TOPAZ. The purpose of this feature is to allow users to explicitly define boundary condition and heat generation relationships by equations rather than by piecewise linear curves. Hence, such things as heat generation by chemical reaction can be modeled. Since TOPAZ3D is a vectorized code, the writing of a user subroutine that is compatible with the main code is not straightforward for novice programmers. Users needing this option should contact the author.

4. EXECUTION

Terminal Execution Line

TOPAZ3D is in the public library MDGLIB on all Cray machines at LLNL. TOPAZ3D is obtained by typing

EXE MDGLIB TOPAZ3D X. / t v

The terminal execution line for TOPAZ3D is as follows:

where

inf = input file

otf = output file (default - TPRINT)

ptf = binary plotting file for graphics (default - TPLOT)

vff = binary viewfactor or exchange factor file

dpf = dump file for restarting (default - TDUMP)

When TOPAZ3D is restarted, the restart input file is optional. The restart input file may be used to redefine output intervals for printed and plotted data, iteration parameters, integration constant, time step size, functional curves and material properties. When restarting from a dump file, the execution line becomes

where

inf = restart input file

rtf = restart file (note - this is the dump file from the previous run)

File name dropouts are permitted, for example

TOPAZ3D I=inf

TOPAZ3D I=inf V=vff

Interactive Controls

Several interactive controls are available to the user when executing TOPAZ3D via terminal. These controls allow the user to query the status of the code execution or to terminate execution. A list of sense switch controls and their corresponding terminal responses follows.

TYPE	RESPONSE
SW1.	A dump file is written and TOPAZ3D terminates.
SW2.	TOPAZ3D responds with time, cycle number and solution convergence information.
SW3.	TOPAZ3D responds every cycle with time, cycle number and solution convergence information until SW3. is retyped.
SW4.	A dump file is written and TOPAZ3D continues calculation.
SW5.	Requests user to input a new time step value and termination time.
SW6.	Requests user to input up to five node numbers whose temperature along with time and cycle number will be printed for succeeding time steps until SW6. is retyped.

5. INPUT DECK

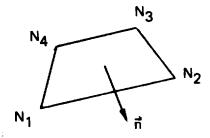
The following "notes" are referenced by number in the data cards that follow.

- Time dependent, temperature dependent, and constant functional relations are indicated by positive, negative, and zero curve numbers respectively. The constant value will be the curve multiplier. Curve numbers greater than 1000 indicate a user subroutine is being provided to evaluate particular functions.
- 2. When data is generated, node or element numbers are incremented according to the sequence.

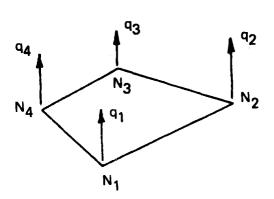
$$N_i, N_i+INC, N_i+2*INC, ..., N_i+NMISS*INC$$

3. When data is generated, the surface numbers, s, are incremented by one following the first number in the sequence and the node numbers are incremented according to

4. By convention, heat flow is positive in the direction of the surface outward normal vector. Surface definition is in accordance with the right hand rule. The outward normal vector points to the right as one progresses from node $N_1-N_2-N_3-N_4$.



5. The curve multiplier on a boundary surface is allowed to vary in a linear fashion by specifying separate values at each corner of the surface.



5.1 Title Card

Columns	Quantity	Format
1-72	Heading to appear on output	12A6
	5.2 Control Cards	
Columns	Card 1 Quantity	Format
1-5	Number of materials (NUMMAT)	15
6-10	Number of nodal points (NUMNP)	15
11-15	Number of elements (NUMEL)	15
16-20	Temperature units (IUNITS) EQ.1: dimensionless EQ.2: centigrade EQ.3: fahrenheit EQ.4: kelvin EQ.5: rankine	I5
21-25	Skip	5x
26-30	Bandwidth and profile minimization (IBAND) EQ.0: no minimization (default) EQ.1: minimization EQ.2: minimization, nodal destination vector is read from input file	15
31-35	Number of function curves used to describe thermal loadings or boundary conditions (NCURV)	15
36-40	Maximum number of points defining any curve (MPCURV)	
41-45	Number of slide surfaces (NSL)	I 5
46-50	Total number of slave nodes (NSLVT)	I 5
51-55	Total number of master nodes (NMSRT)	15
56-60	Node heat flux calculations (IEF) EQ.O: not calculated (default) EQ.1: calculated	15
61-65	Phase change flag EQ.O: no phase change EQ.1: perform phase change calculations	15
66-80	Percentage of available machine memory to use EQ.0: permem = 90.	E15.0

Columns	Quantity	Format
1-5	Number of elements with internal heat generation (NHGEN) $$	15
6-10	Number of nodes at which nonzero initial temperatures are specified (NIT)	15
11-15	Number of nodes at which temperature boundary conditions are specified (NIBC)	15
16-20	Number of flux boundary condition surfaces (NFBC)	15
21-25	Number of convection boundary condition surfaces (NCBC)	15
26-30	Number of radiation boundary condition surfaces (NRBC)	15
31-35	Number of enclosure radiation surfaces (NRSEG)	15
36-40	Number of radiation bands (NBAND)	15
41-45	Number of emissivity vs. wavelength curves (NECURV)	15
46-50	Radiation calculation type (IRTYP) EQ.1: view factors EQ.2: exchange factors	15
51-55	Number of special internal boundary elements (NIBC)	15
56-60	Number of bulk nodes (NBN)	15
61-65	Number of bulk node boundary surfaces (NBNSEG)	15
75-80	Special user RC	15

Card 3

Columns	Quantity	Format
1-5	Analysis type (ITRAN) EQ. 0: steady state EQ. 1: transient	15
Define the	following variables for a transient analysis:	
6-10	Time step code (ISTEP) EQ.0: fixed time step EQ.1: variable time step	15
11-15	Number of time steps between printed data output (IPRINT) EQ.0: default set to 1	15
16-20	Number of time steps between plotted data output (IPLOT) EQ.O: default set to 1	15
21-25	Number of time steps between dump file generation EQ.O: dump file written when TOPAZ3D terminates normally.	15
26-35	Time integration parameter (ALPHA) EQ.O: default set to = 0.5	E10.0

 $\frac{\text{Card 4}}{\text{(If steady-state solution, leave this card blank.)}}$

Fixed-Time Step (ISTEP = 0)

Columns	Quantity	Format
1-10	Initial problem time (TIMIN)	E10.0
11-20	Final problem time (TIMEND)	E10.0
21-30	Time step size (DT)	E10.0
	Variable Time Step (ISTEP = 1)	
Columns	Quantity	<u>Format</u>
1-10	Initial problem time (TIMIN)	E10.0
11-20	Final problem time (TIMEND)	E10.0
21-30	<pre>Initial time step size (DT) EQ.0: default set to 1% of the smallest time constant in the system</pre>	E10.0
31-40	Minimum time step (DTMIN) EQ.O: default set to 1% of the smallest time constant in the system	E10.0
41-50	Maximum time step (DTMAX) EQ.O: default set to 100 times the smallest time constant in the system	E10.0
51-60	Desired maximum temperature change in each time step above which time step will be decreased EQ.0: default set to 1	E10.0
61-70	Modification factor for increasing/decreasing time step EQ.O: default set to 2	E10.0

Card 5

Columns	Quantity	Format
1-5	Type of problem EQ.0: linear problem EQ.1: nonlinear problem	15
Define the	following variables for a nonlinear problem:	
6-10	Number of time steps between conductance matrix reformations EQ.0: default set to 1	15
11-15	Number of time steps between equilibrium iterations EQ.0: default set to 1	15
16-20	Maximum number of conductance matrix reformations per time step EQ.O: default set to 10	15
21-25	Maximum number of equilibrium iterations permitted per conductance matrix reformation EQ.O: default set to 1	15
26-35	Convergence tolerance for equilibrium iterations EQ.O: default set to 0.0001	E10.0
36-45	Relaxation parameter E0.0: default set to 1.	E10.0

5.3 Material Property Data Cards

Repeat the following cards for each material:

Card 1

Columns	Quantity	Format
1-5	Material identification number	15
6-10	Material type EQ.1: isotropic - define only k ₁ EQ.2: isotropic temperature dependent EQ.3: orthotropic - define k ₁ , k ₂ , and k ₃ EQ.4: orthotropic temperature dependent	15
11-20	Density	E10.0
21-30	Temperature at which latent heat is absorbed or released	E10.0
31-40	Latent heat	E10.0
41-45	Thermal generation rate curve number (Note 1)	15
46-55	Thermal generation rate multiplier	E10.0
56-60	For orthotropic material define material axes option, AOPT EQ.0: Locally orthotropic with material axes by element nodes N ₁ ,N ₂ and N ₄ . EQ.1: Locally orthotropic with material axes determined by a point in space and global location of element center. EQ.2: Globally orthotropic with material axes determined by vectors.	15
	Card 2	
Columns	Quantity	Format
1-72	Material identification name	

Material Type 1 - Istropic

Card	Columns	Quantity	Format
3	1-10	Heat Capacity: c	E10.0
	11-20	Thermal conductivity: k	E10.0
4		Blank	
5		Blank	
6		Blank	
7		Blank	
8		Blank	
9		Blank	

Material Type 2 - Isotropic Temperature Dependent

Card	Columns	Quantity	Format
3	1-80	Temperature: $T_1, T_2, \dots T_8$	8E10.0
4	1-80	Heat capacity: $c_1, c_2, \ldots c_8$	8E10.0
5	1-80	Thermal Conductivity: $k_1, k_2, \dots k_8$	8E10.0
6		Blank	
7		Blank	
8		Blank	
9		Blank	

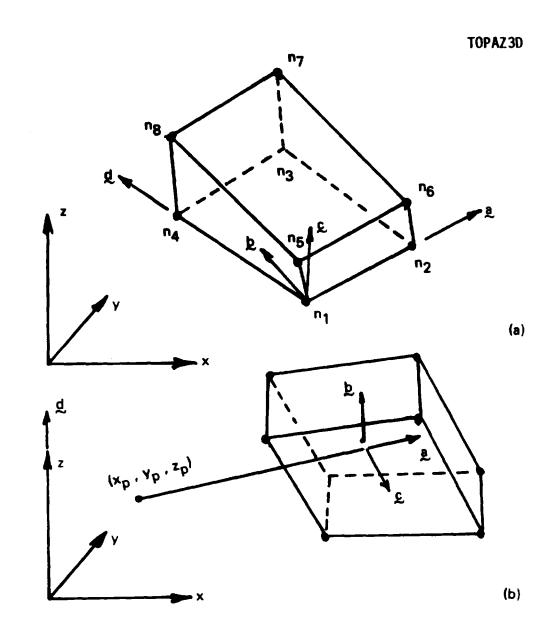
TOPAZ3D

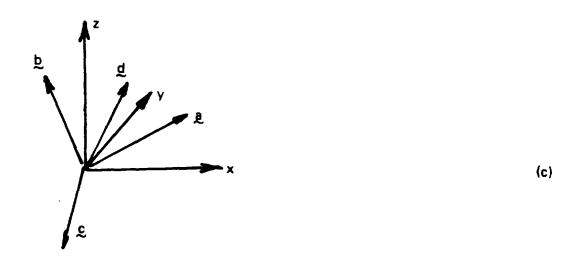
Material Type 3 - Orthotropic

<u>Card</u>	Columns	Quantity	Format
3	1-10	Heat Capacity	E10.0
	11-20	Thermal Conductivity k ₁	E10.0
	21-30	Thermal Conductivity k ₂	E10.0
	31-40	Thermal Conductivity k ₃	E10.0
4		Blank	
5		Blank	
6		Blank	
7		Blank	
8	1-10	x_p , define for AOPT = 1.0	E10.0
	11-20	y_p , define for AOPT = 1.0	E10.0
	21-30	z_p , define for AOPT = 1.0	E10.0
8	1-10	a_1 , define for AOPT = 2.0	E10.0
	11-20	a_2 , define for AOPT = 2.0	E10.0
	21-30	a_3 , define for AOPT = 2.0	E10.0
9	1-10	d_1 , define for AOPT = 2.0	E10.0
	11-20	d ₂ , define for AOPT = 2.0	E10.0
	21-30	d_3 , define for AOPT = 2.0	E10.0

Material Type 4 - Orthotropic Temperature Dependent

Card	Columns	Quantity	Format
3	1-80	Temperature: T ₁ , T ₂ ,T ₈	8E10.0
4	1-80	Heat capacity: C ₁ , C ₂ ,C ₈	8E10.0
5	1-80	Thermal conducitvity: $(k_1)_1, (k_1)_2, \dots (k_1)_8$	8E10.0
6	1-80	Thermal conductivity: $(k_2)_1,(k_2)_2,(k_3)_8$	8E10.0
7	1-80	Thermal conductivity: $(k_3)_1,(k_3)_2,(k_3)_8$	8E10.0
8	1-10	x_p , define for AOPT = 1.0	E10.0
	11-20	y _p , define for AOPT = 1.0	E10.0
	21-30	z _p , define for AOPT = 1.0	E10.0
8	1-10	a_1 , define for AOPT = 2.0	E10.0
	11-20	a_2 , define for AOPT = 2.0	E10.0
	21-30	a_3 , define for AOPT = 2.0	E10.0
9	1-10	d_1 , define for AOPT = 2.0	E10.0
	11-20	d_2 , define for AOPT = 2.0	E10.0
	21-30	d_3 , define for AOPT = 2.0	E10.0





Options for determining principal material axes: (a) AOPT = 0.0, (b) AOPT = 1.0, and (c) AOPT = 2.0. Note that $c = a \times d$ and that $b = c \times a$.

5.4 Nodal Point Cards

Columns	Quantity	<u>Format</u>
1-5	Node point number, N _i	15
6-10	Generation increment	15
11-30	x coordinate	E20.0
31-50	y coordinate	E20.0
51-70	z coordinate	E20.0
71-80	Temperature initial condition	E10.0

Node point cards must be in ascending order if data is to be generated between cards. When data is missing, node numbers are generated according to the sequence

$$N_i, N_i + INC, N_i + 2 \times INC, \dots, N_j$$

where N_{ij} and N_{ij} are the node numbers on two consecutive cards and INC is read from the N_{ij} card. Linear interpolation is used to calculate the coordinates of the generated nodes. If INC is zero or blank, no nodes are generated.

5.5 Element Data Cards

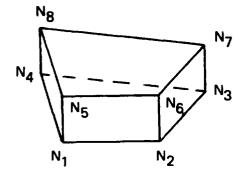
Columns	Quantity	<u>Format</u>
1-5	Element number	15
6-10	Material number	15
11-15	Generation increment (INC)	15
16-55	Node numbers N_1 - N_8	815
56-60	NMISS	15

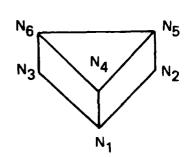
Element cards are assumed to be in element number sequence. Omitted data is automatically generated with respect to the first card prior to the omitted data as follows:

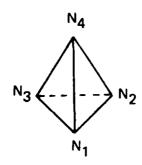
$$N_j^{e+1} = N_j^e + INC$$

The material properties for the generated elements and the mesh generation parameter INC are taken from the first card. The default value of INC is 1.

Nodal points N_1 - N_8 define the corner nodes of the 8-node solid elements. Elements having fewer than 8 nodes are obtained by repeating one or more nodes. Four, six, and eight node elements are shown below. Input of nodes on the element cards for these elements would take the form







5.6 Interface Data Cards

Control Cards Define a control card for each interface

Columns	Quantity	
1-5	Number of slave surfaces in this surface	15
6-10	Number of master surfaces in this surface	15
11-15	Skip	5 X
16-25	Thermal contact resistance	E10.0

Surface Definition Cards

Repeat the following set of cards for each interface

Slave segment cards:

Columns	Quantity	Format
1-5	Slave surface number	15
6-10	Skip	5X
11-30	Node numbers n_1 , n_2 , n_3 , n_4	415
Master seg	ment cards:	
1-5	Master surface number	15
6-10	Skip	5X
11-30	Node numbers n_1 , n_2 , n_3 , n_4	415

5.7 Element Heat Generation Cards

Columns	Quantity	<u>Format</u>
1-5	Element number	15
6-10	Curve number for heat generation rate, $q'''(Note\ 1)$	15
11-20	Curve multiplier for q'''	E10.0
21-25	Number of elements to be generated following this one	15
26-30	Generation increment (INC), (Note 2)	15

5.8 Temperature Initial Condition Cards

Columns	Quantity	Format
1-5	Node number	15
6-15	Initial temperature	E10.0
16-20	Number of nodes to be generated following this one (NMISS)	15
21-25	Generation increment (INC), (Note 2)	15

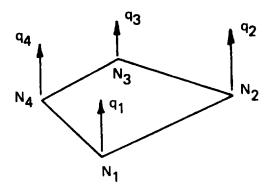
TOPAZ3D

5.9 Temperature Boundary Condition Cards

Columns	Quantity	<u>Format</u>
1-5	Node number	15
6-10	Time function curve number	15
11-20	Curve multiplier	E10.0
21-25	Number of nodes to be generated following this one (NMISS)	15
26-30	Generation increment (INC), (Note 2)	15

5.10 Flux Boundary Condition Cards

Columns	Quantity	<u>Format</u>
1-5	Flux surface number	15
6-25	Node numbers $N_1 - N_4$ (Note 4)	415
26-30	Flux curve number (Note 1)	15
31-70	Curve multipliers at nodes $N_1 - N_4$ (Note 5)	4 E10.0
71-75	Number of surfaces to be generated (NMISS)	15
76-80	Generation increment (INC), (Note 3)	15



5.11 Convection Boundary Condition Cards

Columns	Quantity	Format
1-5	Convection surface number	15
6-25	Node numbers $N_1 - N_4$ (Note 4)	415
26-30	Curve number for h (Note 1)	15
31-40	Curve multiplier for h	E10.0
41-45	Curve number for T_{∞} (Note 1)	15
46-55	Curve multiplier for T $_{\infty}$	E10.0
56-65	Free convection exponent	E10.0
66-70	Number of surfaces to be generated (NMISS)	15
71-75	Generation increment (INC), (Note 3)	I 5

SIMPLIFIED CORRELATIONS FOR AIR [13]

Geometry	Flow	h [W/m ² C]
Horizontal Plates		
 a) Upper surface heated or lower surface cooled 	Turbulent	$h = 1.52 \Delta T^{1/3}$
	Laminar	$h = 1.32 \left(\frac{\Delta T}{L}\right)^{1/4}$
b) Upper surface cooled or lower surface heated	Laminar	$h = 0.59 \left(\frac{\Delta T}{L}\right)^{1/4}$
Horizontal cylinders	Turbulent	$h = 1.24 \Delta T^{1/3}$
	Laminar	$h = 1.32 \left(\frac{\Delta T}{D}\right)^{1/4}$
Vertical plates and cylinders	Turbulent	$h = 1.31 \Delta T^{1/3}$
	Laminar	$h = 1.42 \left(\frac{\Delta^{T}}{L}\right)^{1/4}$

5.12 Radiation Boundary Condition Cards

Columns	Quantity	Format
1-5	Radiation surface number	15
6-25	Node numbers N ₁ - N ₄ (Note 4)	415
26-30	Curve number for f (Note 1)	15
31-40	Curve multiplier for f	E10.0
41-45	Curve number for T $_{\infty}$ (Note 1)	15
46-55	Curve multiplier for T $_{\infty}$	E10.0
56-60	Number of surfaces to be generated (NMISS)	15
61-65	Generation increment (INC), (Note 3)	15

5.13 Enclosure Radiation Data Cards

Card 1

Columns	Quantity	Format
1-10	Stefan-Boltzmann constant	E10.0
Define the	following variables if NBAND > 1:	
11-20	Radiosity convergence tolerance (default - 1.E-04)	E10.0
21-25	Maximum number of radiosity iterations (default = 100)	15

Card 2
(Repeat these cards until all radiation surfaces are defined.)

Columns Quantity Format 1-5 Surface number I 5 6-25 Node numbers $N_1 - N_4$ (Note 4) 415 26 - 30Skip 5X 31-35 Number of surfaces to be generated following this 15 one (NMISS) 36-40 Generation increment (INC), (Note 3) I 5 41-45 Does surface participate in conduction part of 15 problem EQ.O: participation EQ.1: no participation 46-50 Curve number for emissivity 15 51-60 Temperature of surface if curve number = 0 E10.0

Emissivity of surface set to 1

Card 3

Columns	Quantity	Format
1-10	Wavelength breakpoint λ_1	E10.0
11-20	Wavelength breakpoint λ_2	E10.0
71-80	Wavelength breakpoint λ_8	E10.0

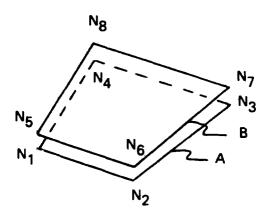
Card 4 (Repeat 'NECURY' times)

Columns	Quantity	<u>Format</u>
1-10	Emissivity for band $0. \rightarrow \lambda_1$	E10.0
11-20	Emissivity for band $\lambda_1 \rightarrow \lambda_2$	E10.0
	•	
	•	
	•	
71-80	Emissivity for band $\lambda_7 \rightarrow \lambda_8$	E10.0

5.14 Special Internal Element Cards

Columns	Quantity	Format
1-40	Node numbers $N_1 - N_8$	815
41-45	Number of elements to be generated following this one (NMISS)	15
46-50	Generation increment (INC)	15
51-60	Curve number for coefficient f (Note 1)	15
61-70	Curve multiplier for f	E10.0
71-75	Exponent "a"	15
76-80	Exponent "b"	15

Eight nodes are required to define an internal boundary element. These nodes should be numbered as shown in the following figure:



Surface A should be defined by nodes N $_1$ -N $_4$ and surface B by nodes N $_5$ -N $_8$. No two node numbers may be the same. However, opposing nodes (e.g. N $_1$ and N $_5$) can have the same coordinates.

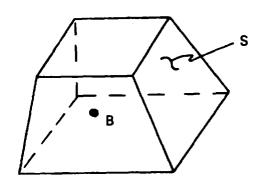
5.15 Bulk Node Data Cards

Card 1

Columns	Quantity	Format
1-5	Bulk node number	15
6-10	Material number of bulk node	15
11-15	Number of boundary surfaces associated with this bulk node: $\mbox{NBSEG}(I)$	15
16-25	Total volume associated with this bulk node	E10.0

 $\frac{\text{Card 2}}{\text{(Omit if NBSEG(I) = 0)}}$

Columns	Quantity	Format
1-20	Node numbers $N_1 - N_4$ (Note 4)	415
21-25	Curve number for coefficient f (Note 1)	15
26-35	Curve multiplier for f	E10.0
36-45	Exponent "a"	E10.0
46-55	Exponent "b"	E10.0
56-60	Number of surfaces to be generated (NMISS)	15
61-65	Generation increment (INC), (Note 3)	15



5.16 Function Curves

(Repeat the following for each curve.)

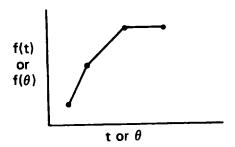
Columns	Quantity	<u>Format</u>
1-5	Curve number	15
6-10	Number of points in curve (NP)	15
11-20	Curve identification	A10

Card 2
(Repeat for NP points.)

Columns	Quantity	Format
1-10	Time or temperature (Note 1)	E10.0
11-20	Function value	E10.0

Curve point coordinates must be in ascending order, starting with the lowest time or temperature.

Values of a function at intermediate points on a curve are obtained by linear interpolation. Functional values outside the range of a curve result in an error message and problem termination (see Section 3.18 RESTART CAPABILITY).



6. RESTART INPUT DECK

A restart input deck is generally not needed to restart TOPAZ. It may be used, however, to reset the following parameters:

- analysis type,
- number of additional time steps,
- time step size,
- output printing and plotting interval,
- integration constant,
- nonlinear iteration parameters,
- function curves,
- material properties.

An entry of 0 or a blank will cause no change in the specified parameter from the previous run unless otherwise noted. All changes made when restarting will be reflected in the next dump file.

Control Card

Columns	Quantity	Format
1-5	Analysis type change flag (IACF)	15
	EQ.0: no change	
	EQ.1: changed as specified below	
6-10	Nonlinear solution parameter change flag (NONLIN)	15
	EQ.0: no change	
	EQ.1: changed as specified below	
11-15	Number of materials to be redefined (NUMAT)	15
16-20	Number of thermal loading curves to be redefined (NUMCUR)	15

Analysis Type Change Cards

Omit these cards if IACF = 0.

Card 1

Columns	Quantity Quantity	Format
1-5	Time step code (ISTEP)	15
	EQ.0: fixed time step	
	EQ.1: variable time step	
6-10	Number of time steps between printed data output (IPRNT)	15
11-15	Number of time steps between plotted data output (IPLOT)	15
16-20	Number of time steps between dump file generation	15
21-30	Time integration parameter (ALPHA)	E10.0

 $\frac{\text{Card 2}}{\text{Fixed Time Step (ISTEP=0)}}$

Columns	Quantity	<u>Format</u>
1-10	Final problem time (TIMEND)	E10.0
11-20	Time step size (DT)	E10.0
	Variable Time Step (ISTEP=1)	
Columns	Quantity	Format
1-10	Final problem time (TIMEND)	E10.0
11-20	Time step size (DT)	E10.0
21-30	Minimum time step (DTMIN)	E10.0
31-40	Maximum time step (DTMAX)	E10.0
41-50	Desired maximum temperature change in each time step above which time step will be decreased	E10.0
51-60	Modification factor for increasing/decreasing time step	E10.0

Nonlinear Solution Parameter Change Card

Omit this card if NONLIN=0

Columns	Quantity	
1-5	Number of time steps between conductance matrix reformations	15
6-10	Number of time steps between equilibrium iterations	15
11-15	Maximum number of conductance matrix reformations per time step	15
16-20	Maximum number of equilibrium iterations permitted per conductance matrix reformation	15
21-30	Convergence tolerance for equilibrium iterations	E10.0
31-40	Relaxation parameter	E10.0

Material Property Change Cards

Skip these cards if NUMAT is equal to zero; otherwise, enter data for NUMAT materials as in Section 5.3. The number of materials redefined (NUMAT) cannot exceed the number of materials specified in the original input.

Function Curve Change Cards

Skip these cards if NUMCUR equals zero; otherwise, define NUMCUR card sets. The number of points in the curve may not change from the original input.

	Card 1	
Columns	Quantity	<u>Format</u>
1-5	Curve number of function curve to be redefined	15
	Card 2	
Columns	Quantity	<u>Format</u>
1-10	Time or temperature E10.0	
11-20	Functional value E10.0	

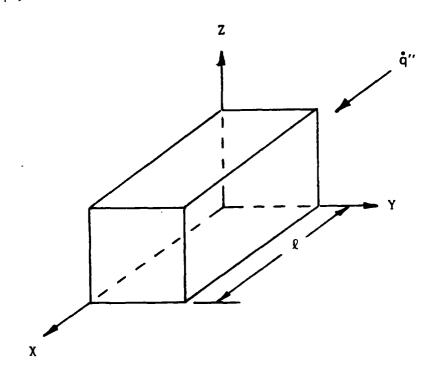
-54-

7. EXAMPLE

Slab with Nonlinear Material Properties

Stewart and Wessling [12] analytically solved the following problem to be used for comparison in validating heat transfer computer codes. They found that several of the computer codes investigated did not correctly handle strong material nonlinearities.

The problem consists of a homogeneous, isotropic slab of finite thickness, ℓ , heated on the front face by a constant and uniform heat flux, $\dot{q}^{"}$, and insulated on the rear face.



The appropriate form of the heat conduction equation is

$$\frac{\partial}{\partial x} (k \frac{\partial T}{\partial x}) = \rho c \frac{\partial T}{\partial t}$$

subject to the initial and boundary conditions

$$T(x,0) = T_0$$

$$\frac{\partial T}{\partial x} (0,t) = -\dot{q}'' / k$$

$$\frac{\partial T}{\partial x} (\ell,t) = 0$$

This problem can be solved analytically for the special case k = k(T), c = c(T), and $\rho = \rho(T)$ such that $k/\rho c = \alpha = constant$. The solution is

$$\frac{\beta T_0 \theta^2}{2} + \theta = \frac{\dot{q}^{"} \ell}{k_0 T_0} \left[\frac{X^2}{2} - X + \frac{1}{3} + Fo - \frac{2}{\pi^2} \right] \sum_{n=1}^{\infty} \frac{1}{n^2} \cos n\pi X e^{-Fo n^2 \pi^2}$$

where

$$\theta = \frac{1 - 1_0}{10}$$

$$\chi = \frac{x}{\varrho}$$

Fo =
$$\frac{\alpha t}{\sigma^2}$$
.

A hypothetical material was chosen with properties

$$\rho = 500 \text{ 1b/ft}^3$$

$$k(T) = k_0 [1 + \beta(T-T_0)] = 1.00 [1 + .005(T-530)]$$
 Btu/hr ft R

$$c(T) = c_0 [1 + \beta(T-T_0)] = 0.05 [1 + .005(T-530)] Btu/lb_m R$$

Other chosen parameters were

$$\dot{q}'' = 2.52 * 10^5 8 tu/hr ft^2$$

$$\ell = 0.03133 \text{ ft}$$

$$T_0 = 530 R$$

$$\beta = 0.005 \, 1/R$$

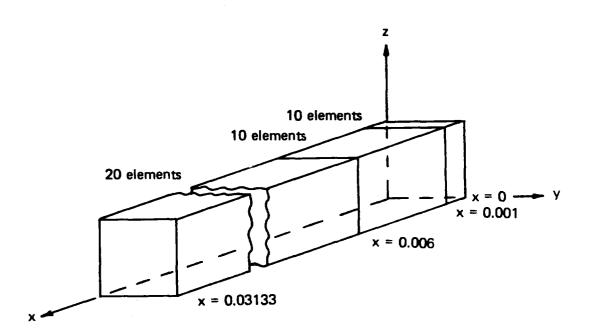
$$k_0 = 1$$
. Btu/hr ft R

$$c_0 = 0.05 \text{ Btu/Lh R}$$

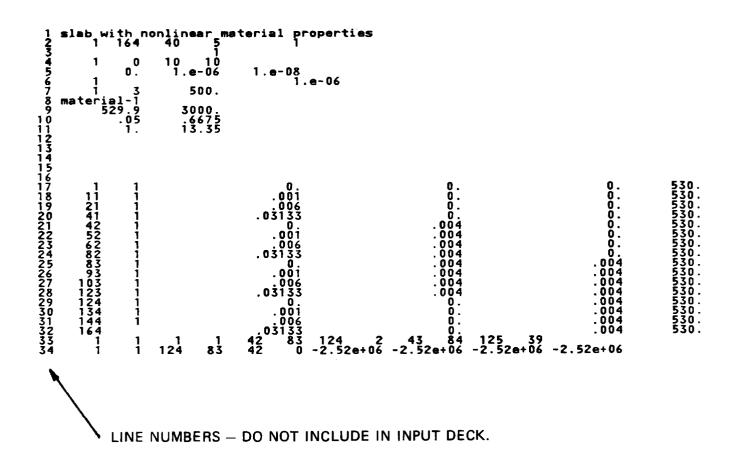
The finite element mesh consisted of 40 elements in the z-direction as shown below. The problem is made one-dimensional by making the sides parallel to the z-axis adiabatic. This is the default boundary condition in TOPAZ3D and does not need to be explicitly defined. By trial-and-error, it was found that fewer elements could not resolve the large temperature gradients existing in this problem. The following table shows the analytical and numerical results for the temperature on the face at x = 0 at various times. The finite element mesh and input listing follow.

TEMPERATURE [R] at x = 0

	TIME [hr]	ANALYTICAL	TOPAZ
1×10^{-6}	874.19	845.44	
1×10^{-5}	1201.41	1200.24	
1×10^{-4}	1851.45	1850.43	



INPUT



TOPAZ3D

8. ACKNOWLEDGEMENT

Special thanks is due Nikki Falco of the Methods Development Group who skillfully typed this report and attended to all the details of getting it printed and distributed.

TOPAZ3D

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